

=> d his

(FILE 'HOME' ENTERED AT 10:30:43 ON 14 MAR 2008)

FILE 'REGISTRY' ENTERED AT 10:30:50 ON 14 MAR 2008

L1 STRUCTURE UPLOADED

L2 0 S L1

L3 17 S L1 FULL

FILE 'CAPLUS' ENTERED AT 10:31:47 ON 14 MAR 2008

L4 19 S L3

L5 19 S L4 AND PY<=2006

FILE 'REGISTRY' ENTERED AT 10:45:37 ON 14 MAR 2008

L6 STRUCTURE UPLOADED

L7 0 S L6

L8 14 S L6 FULL

FILE 'REGISTRY' ENTERED AT 10:46:50 ON 14 MAR 2008

FILE 'CAPLUS' ENTERED AT 10:46:53 ON 14 MAR 2008

L9 10 S L8

FILE 'REGISTRY' ENTERED AT 10:54:53 ON 14 MAR 2008

L10 STRUCTURE UPLOADED

L11 6 S L10

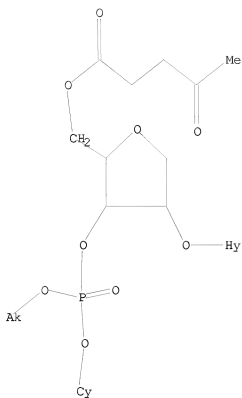
L12 125 S L10 FULL

FILE 'CAPLUS' ENTERED AT 10:56:13 ON 14 MAR 2008

L13 19 S L12

=> d stat que

L10 STR



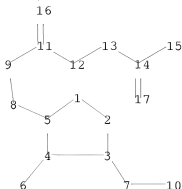
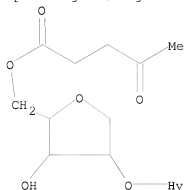
Structure attributes must be viewed using STN Express query preparation.

L12 125 SEA FILE=REGISTRY SSS FUL L10

L13 19 SEA FILE=CAPLUS ABB=ON PLU=ON L12

=>

Uploading C:\Program Files\Stnexp\Queries\10597445-14Mar08-1.str



chain nodes :

6 7 8 9 10 11 12 13 14 15 16 17

ring nodes :

1 2 3 4 5

chain bonds :

3-7 4-6 5-8 7-10 8-9 9-11 11-12 11-16 12-13 13-14 14-15 14-17

ring bonds :

1-2 1-5 2-3 3-4 4-5

exact/norm bonds :

1-2 1-5 2-3 3-4 3-7 4-5 4-6 7-10 9-11 11-16 14-17

exact bonds :

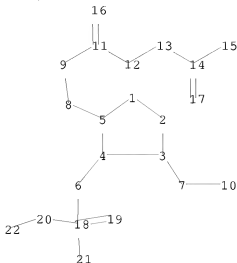
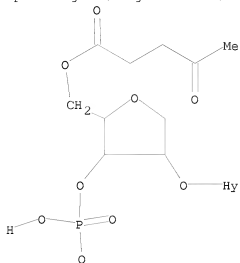
5-8 8-9 11-12 12-13 13-14 14-15

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:CLASS 7:CLASS 8:CLASS 9:CLASS 10:Atom
11:CLASS 12:CLASS 13:CLASS 14:CLASS 15:CLASS 16:CLASS 17:CLASS

=>

Uploading C:\Program Files\Stnexp\Queries\10597445-14Mar08-.str



chain nodes :

6 7 8 9 10 11 12 13 14 15 16 17 18 19 20 21 22

ring nodes :

1 2 3 4 5

chain bonds :

3-7 4-6 5-8 6-18 7-10 8-9 9-11 11-12 11-16 12-13 13-14 14-15 14-17

18-19

18-20 18-21 20-22

ring bonds :

1-2 1-5 2-3 3-4 4-5

exact/norm bonds :

1-2 1-5 2-3 3-4 3-7 4-5 4-6 6-18 7-10 9-11 11-16 14-17 18-21

exact bonds :

5-8 8-9 11-12 12-13 13-14 14-15 20-22

normalized bonds :

18-19 18-20

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:CLASS 7:CLASS 8:CLASS 9:CLASS 10:Atom

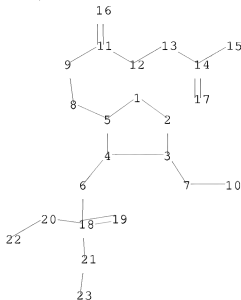
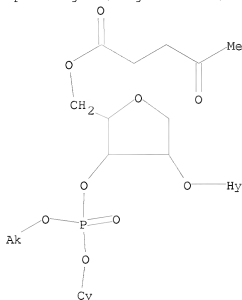
11:CLASS 12:CLASS 13:CLASS 14:CLASS 15:CLASS 16:CLASS 17:CLASS 18:CLASS

19:CLASS 20:CLASS

21:CLASS 22:CLASS

=>

Uploading C:\Program Files\Stnexp\Queries\10597445-14Mar08-3.str



```

chain nodes :
6 7 8 9 10 11 12 13 14 15 16 17 18 19 20 21 22 23
ring nodes :
1 2 3 4 5
chain bonds :
3-7 4-6 5-8 6-18 7-10 8-9 9-11 11-12 11-16 12-13 13-14 14-15 14-17
18-19
18-20 18-21 20-22 21-23
ring bonds :
1-2 1-5 2-3 3-4 4-5
exact/norm bonds :
1-2 1-5 2-3 3-4 3-7 4-5 4-6 6-18 7-10 9-11 11-16 14-17 18-19 18-20
18-21 20-22 21-23
exact bonds :
5-8 8-9 11-12 12-13 13-14 14-15

```

Match level :

```

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:CLASS 7:CLASS 8:CLASS 9:CLASS 10:Atom
11:CLASS 12:CLASS 13:CLASS 14:CLASS 15:CLASS 16:CLASS 17:CLASS 18:CLASS
19:CLASS 20:CLASS
21:CLASS 22:CLASS 23:Atom

```

=> d his

(FILE 'HOME' ENTERED AT 07:52:07 ON 17 MAR 2008)

FILE 'REGISTRY' ENTERED AT 07:52:22 ON 17 MAR 2008

E LIPASE/CN

L1 1 S E3
L2 1 S E3 FULL

FILE 'CAPLUS' ENTERED AT 07:52:53 ON 17 MAR 2008

L3 35400 S L2
L4 5363 S LEVULIN?
L5 104 S LEVULINOYL
L6 1327 S LEVULINATE
L7 4043 S LEVULINIC ACID
L8 4884 S L5 OR L6 OR L7
L9 1 S L2 (S) L8
L10 1 S L2 (L) L8
L11 16 S L2 AND L8

=> d stat que

L2 1 SEA FILE=REGISTRY ABB=ON PLU=ON LIPASE/CN
L5 104 SEA FILE=CAPLUS ABB=ON PLU=ON LEVULINOYL
L6 1327 SEA FILE=CAPLUS ABB=ON PLU=ON LEVULINATE
L7 4043 SEA FILE=CAPLUS ABB=ON PLU=ON LEVULINIC ACID
L8 4884 SEA FILE=CAPLUS ABB=ON PLU=ON L5 OR L6 OR L7
L11 16 SEA FILE=CAPLUS ABB=ON PLU=ON L2 AND L8

```

FILE 'CASREACT' ENTERED AT 11:11:30 ON 20 MAR 2008
L1      STRUCTURE UPLOADED
L2      0 S L1
L3      0 S L2 FULL
L4      0 S L1 FULL
L5      STRUCTURE UPLOADED
L6      0 S L5
L7      0 S L5 FULL

FILE 'STNGUIDE' ENTERED AT 11:14:52 ON 20 MAR 2008

FILE 'REGISTRY' ENTERED AT 11:16:14 ON 20 MAR 2008
E 2-CHLOROPHENYLPHOSPHOROTRIAZOLIDE
E 2-CHLOROPHENYLPHOSPHOROTRIAZOLIDE/CN
E PHOSPHOROTRIAZOLIDE/CN
L8      1668 S CHLORO (XA) PHOSPHORO (XA) PHENYL (XA) TRI
L9      0 S CHLORO (XA) PHOSPHORO (XA) PHENYL (XA) TRIAZOLIDE
L10     197 S CHLORO (XA) PHOSPHORO (XA) PHENYL (XA) TRIAZO?
L11     197 S CHLORO (XA) PHOSPHORO (XA) PHENYL (XA) TRIAZO? (XA) 2

FILE 'CAPLUS' ENTERED AT 11:19:04 ON 20 MAR 2008
E US2007172925/PN
L12     1 S E3

FILE 'REGISTRY' ENTERED AT 11:20:45 ON 20 MAR 2008
L13     1 S 861817-06-3/RN
SET NOTICE 1 DISPLAY
SET NOTICE LOGIN DISPLAY

FILE 'CAPLUS' ENTERED AT 11:21:40 ON 20 MAR 2008
SEL L12 RN

FILE 'REGISTRY' ENTERED AT 11:21:50 ON 20 MAR 2008
L14     85 S E1-E85
L15     3 S L14 AND PHOSPH?

FILE 'CASREACT' ENTERED AT 11:22:47 ON 20 MAR 2008
L16     48 S L15

FILE 'REGISTRY' ENTERED AT 11:26:25 ON 20 MAR 2008
L17     1 S L14 AND TRICHLORO?

FILE 'CASREACT' ENTERED AT 11:27:09 ON 20 MAR 2008
L18     264 S L17
L19     48 S L18 AND PHOSPH?

FILE 'CASREACT' ENTERED AT 11:40:02 ON 20 MAR 2008
L20     9 S L19 AND PHOSPHITE

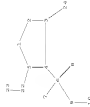
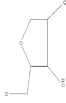
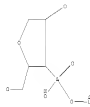
FILE 'STNGUIDE' ENTERED AT 11:50:16 ON 20 MAR 2008

=> d stat que
L14     85 SEA FILE=REGISTRY ABB=ON PLU=ON (100-07-2/BI OR 108-24-7/BI
OR 109-78-4/BI OR 115-20-8/BI OR 118-00-3/BI OR 1191-99-7/BI
OR 120187-92-0/BI OR 120187-94-2/BI OR 138494-30-1/BI OR
21090-30-2/BI OR 40608-06-8/BI OR 40615-36-9/BI OR 40615-37-0/B
I OR 40615-39-2/BI OR 64350-24-9/BI OR 65-46-3/BI OR 69304-37-6
/BI OR 72351-28-1/BI OR 75-77-4/BI OR 79-30-1/BI OR 80817-46-5/
BI OR 85393-37-9/BI OR 861816-91-3/BI OR 861816-92-4/BI OR

```

861816-93-5/BI OR 861816-94-6/BI OR 861816-95-7/BI OR 861816-97-9/BI OR 861816-98-0/BI OR 861816-99-1/BI OR 861817-01-8/BI OR 861817-03-0/BI OR 861817-04-1/BI OR 861817-05-2/BI OR 861817-06-3/BI OR 861817-07-4/BI OR 861817-09-6/BI OR 861817-10-9/BI OR 861817-11-0/BI OR 861842-82-2/BI OR 861842-83-3/BI OR 861842-85-5/BI OR 861842-86-6/BI OR 861842-87-7/BI OR 861842-88-8/BI OR 861842-89-9/BI OR 861842-90-2/BI OR 861842-91-3/BI OR 861842-92-4/BI OR 861842-93-5/BI OR 861842-95-7/BI OR 861842-96-8/BI OR 861842-97-9/BI OR 861842-98-0/BI OR 861842-99-1/BI OR 861843-00-7/BI OR 861843-01-8/BI OR 861843-02-9/BI OR 861843-03-0/BI OR 861843-04-1/BI OR 861843-05-2/BI OR 861843-06-3/BI OR 861843-07-4/BI OR 861843-08-5/BI OR 861843-09-6/BI OR 861843-10-9/BI OR 861843-11-0/BI OR 861843-12-1/BI OR 861843-13-2/BI OR 862202-73-1/BI OR 862224-10-0/BI OR 862224-11-1/BI OR 862224-12-2/BI OR 862224-13-3/BI OR 862224-14-4/BI OR 862224-15-5/BI OR 862224-16-6/BI OR 862224-17-7/BI OR 862224-18-8/BI OR 862259-89-0/BI OR 86327-76-6/BI OR 87865-78-9/BI OR 9001-62-1/BI OR 90865-73-9/BI OR 90865-74-0/BI)

| | | | | |
|-----|-----|--------------------------|--------|--------------------|
| L17 | 1 | SEA FILE=REGISTRY ABB=ON | PLU=ON | L14 AND TRICHLORO? |
| L18 | 264 | SEA FILE=CASREACT ABB=ON | PLU=ON | L17 |
| L19 | 48 | SEA FILE=CASREACT ABB=ON | PLU=ON | L18 AND PHOSPH? |
| L20 | 9 | SEA FILE=CASREACT ABB=ON | PLU=ON | L19 AND PHOSPHITE |



```

chain nodes :
ring nodes: 6 7 8 9 10 16 19 20 21 22 23 24
ring nodes: 4 5 11 12 13 14 15
chain bonds: 3-24 4-6 5-22 6-7 6-8 6-9 9-10 13-19 14-16 15-20 20-21 22-23
ring bonds :
1-2 1-5 2-3 3-4 4-5 11-12 11-15 12-13 13-14 14-15
exact/norm bonds: 2-3 3-4 3-24 4-5 6-9 11-12 11-15 12-13 13-14 14-16 20-21
22-23
exact bonds :
4-6 5-22 9-10 15-20
normalized bonds :
6-7 6-8

```

```

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:CLASS 7:CLASS 8:CLASS 9:CLASS 10:Atom 11:Atom
13:Atom 14:Atom 15:Atom 16:CLASS 19:CLASS 20:CLASS 21:CLASS 22:CLASS 23:CLASS
24:CLASS
fragments assigned product role:
Containing 1
fragments assigned reactant/reagent role:
Containing 11
node 4:14 4:14

```



```

chain nodes :
ring nodes: 7 8 9 10 16
chain bonds: 4 5 11 12 13 14 15
chain bonds: 6-8 6-9 9-10 14-16
ring bonds : 2-3 3-4 4-5 11-12 11-15 12-13 13-14 14-15
exact/norm bonds: 2-3 3-4 4-5 6-9 11-12 11-15 12-13 13-14 14-15 14-16
exact bonds : 4-6 9-10
normalized bonds :
6-7 6-8

```

```

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:CLASS 7:CLASS 8:CLASS 9:CLASS 10:Atom 11:Atom
12:Atom 13:Atom 14:Atom 15:Atom 16:CLASS
resc1:XC 4:16:XC
4:6:XC 14:16:XC

```